

How often does theory match experiment?

Anirban Banerji

Bioinformatics Centre, University of Pune,
Pune-411007, India
anirbanab@gmail.com, anirban@bioinfo.ernet.in

February 12, 2009

Abstract

In every sphere of science, theories make predictions and experiments validate them. However, common experience suggests that theoretically predicted exact magnitude for a parameter, constitute a small subset of all the experimentally obtained magnitudes for that particular parameter. Typically, irrespective of the branch of science and the particular problem under consideration, the set of obtained experimental results form an interval $[x_{min}, x_{max}]$, within which the theoretically predicted magnitude, say x , occurs with time, apparently randomly. We attempt here to find the characteristics of the statistical distribution of events of experimental observation of the occurrence of theoretically predicted x ; in other words, characterization of the time interval when theoretical predictions match the experimental readings, exactly.

Recording the readings from experimental apparatus is ubiquitous in every branch of science. While the theoretical studies help us to predict the expected magnitude that any parameter should own, experiments verify whether the parameters actually assume the predicted magnitudes; and if they don't, by what margin do they differ from the theoretical idealizations. In some of these cases experiments are one-off in nature; whereas in many cases, we gather results from the apparatus in a sequential manner before studying the extent by which the mean and variance of the experimentally obtained data differs from the theoretical predictions (if they do, at all). In case of the later, we collect the results as a sequence of homogeneous events occurring one after another, which implies that the occurrence of results constitute a flow of events. There might or might not be a fixed time interval between the occurrences of these results. In the present work we attempt to understand the nature of the process of observing the occurrences of experimental results, for the general case where they occur without any fixed time interval between them. Since we know it from our experience that the precise magnitude of theoretically predicted result (from a pool of results that differ from the exact expectation by arbitrarily small margin) shows up in the apparatus only now and then and not always;

attempts are made to characterize the time intervals between occurrences of results, when theoretical idealizations match absolutely with the experimental realities (referred to as 'events' from here onwards).

It is not that attempts have not been made to tackle this problem. On the contrary, previous attempts to characterize this problem were many (and they form a spectrum of standpoints); but most of them were qualitative in nature and were only tangentially touching upon the mathematical description of the situation. For example, [1] talks about certain prevalent patterns in experimental observation in particular cases related to states in Alzheimer's disease whereas [2], [3] and [4] had attempted to understand the general philosophical nature of the problem from various perspectives. Although [5] and [6] were objective and quantitative in their basic premise of description, the precise question that we are raising in this work was not addressed. Similarly, although the attempts of [7], [8] and [9] had touched upon the extent to which theoretical predictions matched experimental findings in various experimental cases, the statistical characterization of precise time-intervals between two events where theoretically predicted magnitude for a parameter matches exactly with experimentally obtained values, remained unanswered.

Experience suggests that results are generally produced one at a time, for any arbitrarily small time interval, and not in a group of two, three per time interval; for most of the experiments across the spectrum of scientific streams. This implies that the probability of two or more events occurring in an elementary time interval Δt is negligibly small compared to the probability of single events occurring at different time intervals (arbitrarily chosen); and hence we conclude that the flow of events (when theoretically predicted result matches absolutely with experimentally obtained results) is ordinary [10]. We observe further that the probability characteristic describing the nature of occurrences of these results do not depend upon the choice of some particular reference frame; i.e., the flow of events is stationary [11]. Experience teaches us further that the number of events occurring on any particular time interval, say t_1 , does not, in general, depend upon number of events occurring on any other non-overlapping interval. These characteristics imply that the flow of events (occurrences of results in a sequential manner) can be represented as a stationary Poisson flow [12]. Alongside all of these, a closer look of the problem reveals that in most of the cases, the time intervals T_1, T_2, \dots between successive events are independent. We assume, with no loss of generality, that intervals between T_1, T_2, \dots are similarly distributed random variables. Aforementioned observations and the assumptions tend to suggest that flow of occurrences of results when theoretical prediction matches experimentally obtained results absolutely, can be categorized as a 'recurrent flow' with limited after-effects [13] (in other words, a 'Palm flow'). [14]

We now attempt to describe an extremely familiar situation when an experimentalist is taking the readings to verify his/her prediction (from theoretical studies) about what to expect in terms of exact magnitude of some parameter. In many of the situations like this, the desired events of occurrence of predicted magnitude occurs, but only as an element of a set of produced results, where most of the elements of the set differ from the expected magnitude by a little. Any experimentalist, from any branch of science, is aware of such a situation; but knowledge of any pattern in the occurrences of aforementioned desired results, eludes the students of science.

To describe the situation, we start by assuming that the occurrences of the theoretically predicted result constitute a 'recurrent flow' on the time axis and the intervals between any two occurrences of them, follow a distribution with density $f(t)$. The assumption that the pattern of output generation can be described by $f(t)$ is not unrealistic; because, results occur as an output of a definite, deterministic process (carefully planned experiment, in any branch of science).

We denote the exact moments of occurrence of the events of absolute match between theoretically predicted results and experimentally found ones, by τ . We seek to find the distribution density of $f^\tau(\tau)$ of the interval T^τ , where the points in the time axis τ occur. This implies, calculation of probability where $f^\tau(\tau) dt$ equals that of τ 's occurrence between length of time interval $(t, t + \Delta t)$. Assuming the presence of very large number of intervals (N) between the events constituting the entire temporal extent of the experiment Γ ; we find that the average number of intervals with length in the range $(t, t + \Delta t)$ is $Nf(t)dt$; whereas the average total length of all such intervals equals $tNf(t)dt$. The average total length of all the N intervals on Γ can be represented as Nx_t , where x_t denotes the expectation $E[T] = \int_0^\infty tf(t)dt$. Hence :

$$f^\tau(\tau) dt \approx \frac{tNf(t)dt}{Nx_t} = \frac{tf(t)}{x_t} dt \quad (1)$$

The approximation in eqⁿ1 becomes more exact when longer interval of time Γ is considered (larger N). Distribution of the random variable T^τ can then be found by evaluating the limit,

$$f^\tau(\tau) = \lim_{x_t \rightarrow \infty} \frac{t}{x_t} f(t) (t > 0). \quad (2)$$

$$E[T^\tau] = \lim_{x_t \rightarrow \infty} \frac{1}{x_t} \int_0^\infty t^2 f(t) dt = \frac{1}{x_t} \mu_2(t) = \frac{1}{x_t} (\sigma_t^2 + x_t^2) \quad (3)$$

$$\sigma^2[T^\tau] = \lim_{x_t \rightarrow \infty} \mu_2[T^\tau] - (E[T^\tau])^2 = \lim_{x_t \rightarrow \infty} \frac{1}{x_t} \int_0^\infty t^3 f(t) dt - (E[T^\tau])^2 \quad (4)$$

However, from an experimentalist's point of view, it would be more useful to know the characteristics of the case where any time interval T^τ is divided in two intervals I_1 and I_2 , by the occurrence of the events when theoretically predicted magnitude for some parameter matches with the experimental findings, at a random instance τ . Here I_1 is defined by nearest previous event to τ and I_2 is defined by the occurrence of τ to the nearest successive event. Characterization of such a case will be of immense practical help to the experimentalists.

We approach the situation by assuming $T^\tau = \theta$. By introducing a density $f_{I_1}(t|\theta)$ that describes the conditional probability of the interval I_1 in the presence of θ . We observe that occurrence of the event of exact match between from theoretical prediction and experimentally obtained result, is random in time; and hence we can consider its having a uniform distribution in the interval θ , given by :

$$[f_{I_1}(t|\theta) = \frac{1}{\theta}], \forall 0 < t < \theta \quad (5)$$

However, to find the marginal distribution $f_{I_1}(t)$, we average the density (eqⁿ-5) considering, the weight $f^\tau(\tau)$. Applying eqⁿ-2, we obtain :

$$f^\tau(\theta) = \frac{\theta}{x_t} f(\theta) \text{ and } f_{I_1}(t) = \int_0^\infty f_{I_1}(t|\theta) f^\tau(\theta) d\theta$$

But, since $f_{I_1}(t|\theta)$ is nonzero only for $\theta > t$, we can write

$$f_{I_1}(t) = \int_t^\infty \frac{\theta}{\theta x_t} f(\theta) d\theta = \frac{1}{x_t} \int_t^\infty f(t) dt = \frac{1}{x_t} [1 - \Phi(t)] \quad (6)$$

where $\Phi(t)$ is the distribution function of the interval t between the events in the 'recurrent flow'.

It is evident that I_2 ($I_2 = T^\tau - I_1$), will have the identical distribution :

$$f_{I_2}(t) = \frac{1}{x_t} [1 - \Phi(t)] \quad (7)$$

Conclusion :

With the help of this simple model a construct is proposed that could characterize the mathematical nature of distribution of instances when theoretical prediction about the magnitude of any parameter matches with the experimental results. This distribution is found to resemble the characteristics of a 'recurrent flow' with limited after-effects. Since the number of assumptions involved in constructing this model are kept at a minimal and the possible domain of applicability of the aforementioned finding encompasses the entire gamut of scientific paradigms (wherever the magnitude of any theoretically predicted parameter is

compared with mean and variance of the experimentally obtained results), the model will hopefully serve students of science, across the barriers of scientific streams.

Acknowledgment : This work was supported by COE-DBT(Department of Biotechnology, Govt. of India) scheme.

The author would like to thank the Director of Bioinformatics Centre, University of Pune; Dr. Urmila Kulkarni-Kale and Professor Indira Ghosh(his PhD supervisor), for providing him with the opportunity to perform this work, although it has got nothing to do with his PhD. research.

References :

- [1] Behl C., Oxidative stress in Alzheimer's Disease: Implications for Prevention and Therapy, "Alzheimer's Disease : Cellular and Molecular Aspects of Amyloid β ", Harris JR, Fahrenholz F (Eds.); Springer, USA; 2005, pp 65-78.
- [2] Wuketits F.M. , Functional Realism, "Functional Models of Cognition: Self-organizing Dynamics and Semantic Structures in Cognitive Systems", Arturo Carsetti (Eds), Springer, 1999, pp 27-38.
- [3] McGrath A.E., "Science and Religion: An Introduction", Blackwell Pub, 1999; pp-78.
- [4] Adams G. and Stocks E.L., A Cultural Analysis of the Experiment and an Experimental Analysis of Culture, Social and Personality Psychology Compass, 2 (5), 1895-1912.
- [5] Vasileva L.A. and Gortsev A.M., Estimation of Parameters of a Double-Stochastic Flow of Events under Conditions of Its Incomplete Observability, Automation and Remote Control, 63(3), 2002, 511-515.
- [6] Arita M., Introduction to the ARM Database: Database on Chemical Transformations in Metabolism for Tracing Pathways, "Metabolomics : The Frontier of Systems Biology", Tomita M. and Nishioka T., (Eds), pp 193-210.
- [7] Downs A.J., Himmel H.J and Manceron L., Low valent and would-be multiply bonded derivatives of the Group 13 metals Al, Ga and In revealed through matrix isolation, Polyhedron, 21 (5-6), 2002, 473-488.
- [8] Judd B.R, Complex atomic spectra, 1985, Rep. Prog. Phys., 48, 907-954.
- [9] Ramirez-Duverger A.S., and Llmaz R.G., Light scattering from a multimode waveguide of planar metallic walls, Optics Communications, 227(4-6), 2003, 227-235.
- [10] Kovalenko I.N., Kuznetsov N.Y. and Shurenkov V.M.; Models of Random Processes: A Handbook for Mathematicians and Engineers; 1996; Boca Raton: CRC Press, pp.155
- [11] Ibid. pp-162.
- [12] Ibid. pp-77.
- [13] Kalashnikov, V., Mathematical Methods in Queuing Theory, Springer, 1994, pp-10.
- [14] Kovalenko I.N., Kuznetsov N.Yu. and Shurenkov V.M.; Models of Random Processes: A Handbook for Mathematicians and Engineers; 1996; Boca Raton: CRC Press, pp.161.